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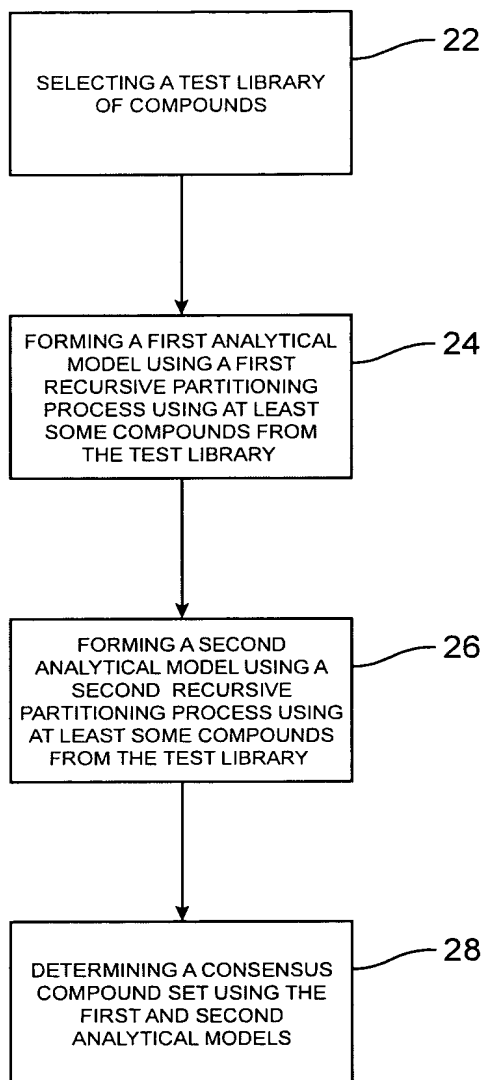


FIG. 1

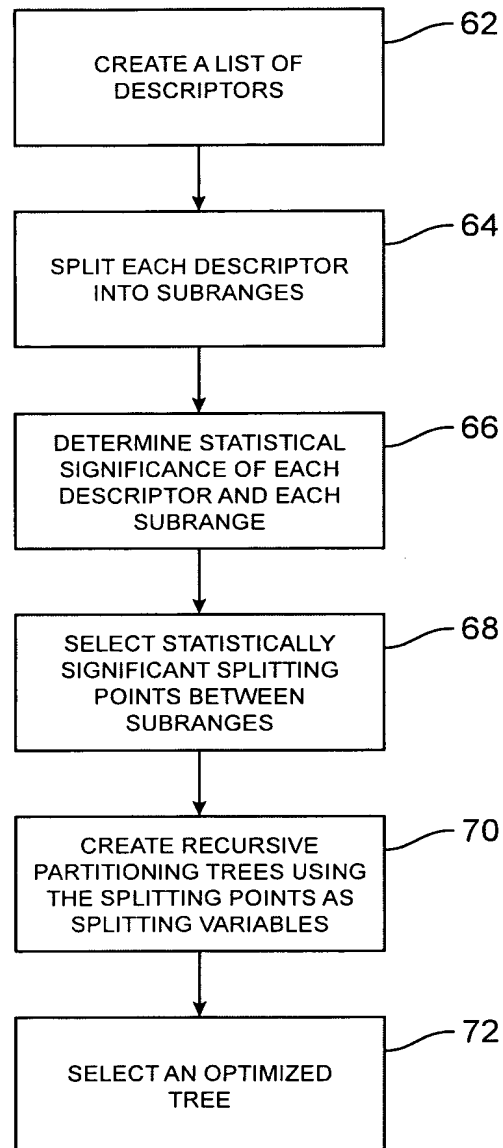


FIG. 2



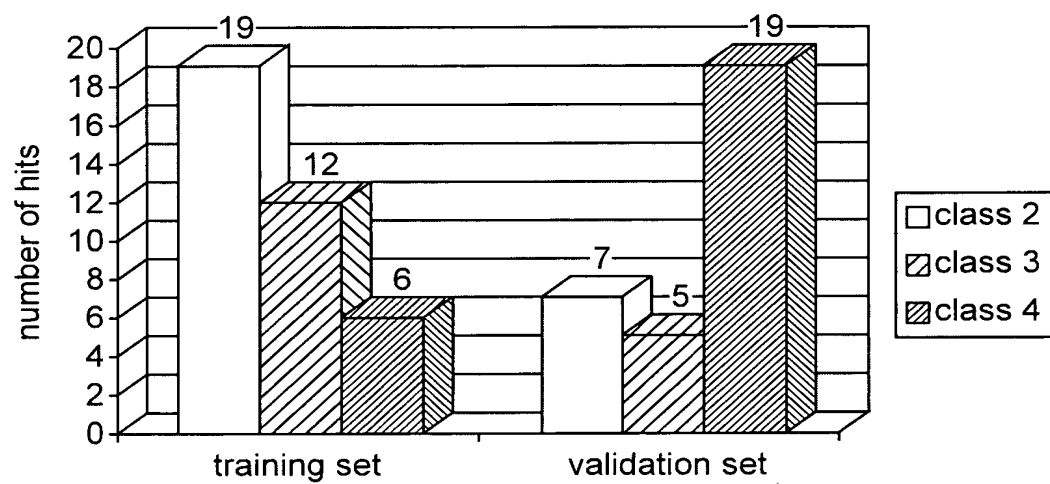


FIG. 4(a)

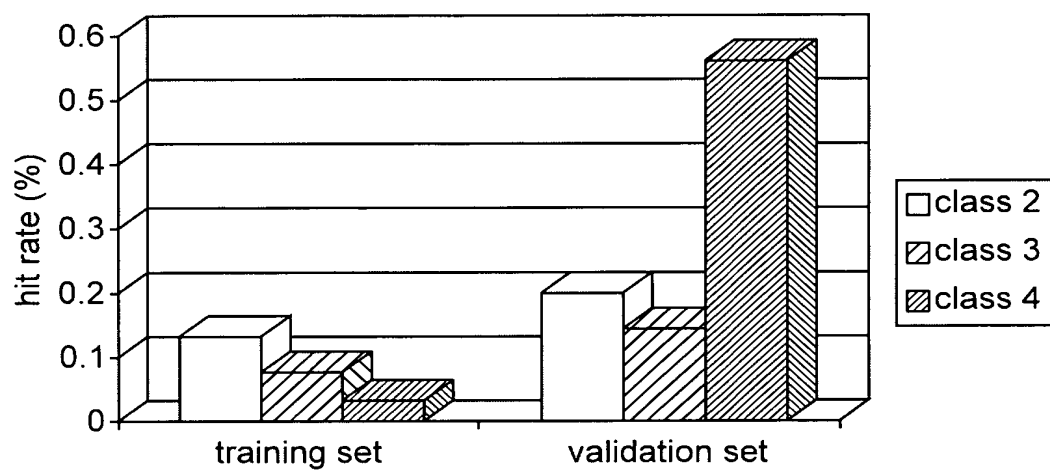


FIG. 4(b)

TABLE I

| TD | max. knots | min. samples | % class correct | fold enrichment | % false positives | # selected | # active nodes | # terminal nodes | selected/node |
|----|------------|--------------|-----------------|-----------------|-------------------|------------|----------------|------------------|---------------|
| 9 | 85 | 144 | 89 | 14.6 | 98.2 | 882 | 5 | 27 | 176.4 |
| 9 | 103 | 90 | 100 | 21.0 | 97.4 | 688 | 7 | 35 | 98.3 |
| 9 | 103 | 54 | 89 | 22.8 | 97.2 | 562 | 7 | 37 | 80.3 |
| 12 | 107 | 18 | 94 | 65.8 | 91.8 | 207 | 9 | 59 | 23.0 |
| 12 | 107 | 3 | 94 | 184.2 | 77.0 | 74 | 11 | 95 | 6.7 |
| 12 | 137 | 1 | 100 | 370.0 | 53.9 | 39 | 13 | 117 | 3.0 |

FIG. 5

TABLE II

| Training Set | | | | | | | | | | | | |
|-------------------|------------|----|------------|--------------|-----------------|-----------------|------|-------|-----------|-----------------|-----------------|-------------------|
| model | descriptor | TD | max. knots | min. samples | % class correct | fold enrichment | cpds | total | consensus | % class correct | fold enrichment | % false positives |
| consensus model 1 | C45 | 9 | 85 | 144 | 89 | 14.6 | 882 | 1245 | 451 | 78 | 24.8 | 96.9 |
| | C45 | 9 | 90 | 144 | 83 | 14.8 | 814 | | | | | |
| consensus model 2 | C45 | 9 | 85 | 144 | 89 | 14.6 | 882 | 1199 | 632 | 83 | 19.0 | 97.6 |
| | C45 | 9 | 80 | 144 | 89 | 13.5 | 949 | | | | | |
| consensus model 3 | C45 | 9 | 80 | 144 | 89 | 13.5 | 949 | 1493 | 411 | 73 | 25.3 | 96.8 |
| | C45 | 9 | 85 | 144 | 89 | 14.6 | 882 | | | | | |
| | C45 | 9 | 90 | 144 | 83 | 14.8 | 814 | | | | | |
| consensus model 4 | C45 | 9 | 85 | 144 | 89 | 14.6 | 882 | 996 | 91 | 83 | 114.3 | 84.6 |
| | C45 | 12 | 107 | 18 | 94 | 65.8 | 207 | | | | | |
| consensus model 5 | C45 | 12 | 107 | 18 | 94 | 65.8 | 207 | 241 | 173 | 94 | 78.6 | 90.2 |
| | C45 | 12 | 109 | 18 | 94 | 65.8 | 207 | | | | | |
| consensus model 6 | C45 | 12 | 107 | 18 | 94 | 65.8 | 207 | 354 | 77 | 94 | 176.6 | 77.9 |
| | C45 | 12 | 127 | 18 | 100 | 64.4 | 224 | | | | | |
| consensus model 7 | C45 | 9 | 85 | 144 | 89 | 14.6 | 882 | 1563 | 165 | 83 | 63.0 | 90.9 |
| | BCUT | 8 | 101 | 144 | 94 | 15.8 | 848 | | | | | |

FIG. 6

TABLE III

| | | | | | | | HTS Eligible | | |
|-------------------|------------|----|------------|--------------|-----------------|-----------------|--------------|--------|-----------|
| model | descriptor | TD | max. knots | min. samples | % class correct | fold enrichment | cpds | total | consensus |
| consensus model 1 | C45 | 9 | 85 | 144 | 89 | 14.6 | 73106 | 155699 | 26354 |
| | C45 | 9 | 90 | 144 | 83 | 14.8 | 68942 | | |
| consensus model 2 | C45 | 9 | 85 | 144 | 89 | 14.6 | 73106 | 168263 | 50449 |
| | C45 | 9 | 80 | 144 | 89 | 13.5 | 105601 | | |
| consensus model 3 | C45 | 9 | 80 | 144 | 89 | 13.5 | 105601 | 235436 | 21821 |
| | C45 | 9 | 85 | 144 | 89 | 14.6 | 73106 | | |
| | C45 | 9 | 90 | 144 | 83 | 14.8 | 68942 | | |
| consensus model 4 | C45 | 9 | 85 | 144 | 89 | 14.6 | 73106 | 94930 | 6241 |
| | C45 | 12 | 107 | 18 | 94 | 65.8 | 28065 | | |
| consensus model 5 | C45 | 12 | 107 | 18 | 94 | 65.8 | 28065 | 46842 | 19720 |
| | C45 | 12 | 109 | 18 | 94 | 65.8 | 25632 | | |
| consensus model 6 | C45 | 12 | 107 | 18 | 94 | 65.8 | 28065 | 60999 | 9987 |
| | C45 | 12 | 127 | 18 | 100 | 64.4 | 30056 | | |
| consensus model 7 | C45 | 9 | 85 | 144 | 89 | 14.6 | 73106 | 127864 | 6309 |
| | BCUT | 8 | 101 | 144 | 94 | 15.8 | 61067 | | |

FIG. 7

TABLE IV

| | | | | | | | Validation Set | | | | | | | |
|-------------------|------------|----|------------|--------------|-----------------|-----------------|----------------|-------|-----------|--------------|--------------|--------------|---------------------------|-------------------------------|
| model | descriptor | TD | max. knots | min. samples | % class correct | fold enrichment | cpds | total | consensus | class 4 hits | class 3 hits | class 2 hits | fold enrichment (class 4) | fold enrichment (class 4 & 3) |
| consensus model 1 | C45 | 9 | 85 | 144 | 89 | 14.6 | 2242 | 2323 | 1351 | 18 | 4 | 5 | 31.7 | 13.0 |
| | C45 | 9 | 90 | 144 | 83 | 14.8 | 1432 | | | | | | | |
| consensus model 2 | C45 | 9 | 85 | 144 | 89 | 14.6 | 2242 | 2342 | 1553 | 18 | 5 | 5 | 27.6 | 11.8 |
| | C45 | 9 | 80 | 144 | 89 | 13.5 | 1653 | | | | | | | |
| consensus model 3 | C45 | 9 | 80 | 144 | 89 | 13.5 | 1653 | 2395 | 1270 | 18 | 4 | 5 | 33.7 | 13.9 |
| | C45 | 9 | 85 | 144 | 89 | 14.6 | 2242 | | | | | | | |
| | C45 | 9 | 90 | 144 | 83 | 14.8 | 1432 | | | | | | | |
| consensus model 4 | C45 | 9 | 85 | 144 | 89 | 14.6 | 2242 | 2267 | 238 | 3 | 3 | 1 | 30.0 | 20.2 |
| | C45 | 12 | 107 | 18 | 94 | 65.8 | 263 | | | | | | | |
| consensus model 5 | C45 | 12 | 107 | 18 | 94 | 65.8 | 263 | 314 | 210 | 2 | 3 | 1 | 22.7 | 19.0 |
| | C45 | 12 | 109 | 18 | 94 | 65.8 | 261 | | | | | | | |
| consensus model 6 | C45 | 12 | 107 | 18 | 94 | 65.8 | 263 | 474 | 92 | 2 | 1 | 1 | 51.8 | 26.1 |
| | C45 | 12 | 127 | 18 | 100 | 64.4 | 303 | | | | | | | |
| consensus model 7 | C45 | 9 | 85 | 144 | 89 | 14.6 | 2242 | 2365 | 421 | 9 | 4 | 4 | 50.9 | 24.7 |
| | BCUT | 8 | 101 | 144 | 94 | 15.8 | 544 | | | | | | | |

FIG. 8